

# Tuning of Zero Energy States in Quantum Dots of Silicene and Bilayer Graphene by Electric Field

Hazem Abdelsalam<sup>a,b,\*</sup>, T. Espinosa-Ortega<sup>c</sup>, Igor Lukyanchuk<sup>a,d</sup>

<sup>a</sup>University of Picardie, Laboratory of Condensed Matter Physics, Amiens, 80039, France

<sup>b</sup>Department of Theoretical Physics, National Research Center, Cairo, 12622, Egypt

<sup>c</sup>Division of Physics and Applied Physics, Nanyang Technological University 637371, Singapore

<sup>d</sup>L. D. Landau Institute for Theoretical Physics, Moscow, Russia

---

## Abstract

Electronic properties of triangular and hexagonal nano-scale quantum dots (QDs) of Silicene and bilayer graphene are studied. It is shown that the low-energy edge-localized electronic states, existing within the size-quantized gap are easily tunable by electric field. The appearance and field evolution of the electronic gap in these zero energy states (ZES) is shown to be very sensitive to QD geometry that permits to design the field-effect scalable QD devices with electronic properties on-demand.

## Keywords:

Silicene; Bilayer Graphene; Zero Energy States; Electric Field; Energy Gap

---

## 1. Introduction

Interest to new graphene-like materials is related with the rising quest to develop the nano-scale field-effect transistor [1, 2], unifying the remarkable electronic properties of graphene with possibility of easy tuning by electric field. Given that the monolayer graphene itself is not quite sensitive to the applied field, the natural way consists in creations of the multi-layer structure with gate-controlled potential difference between layers. Two systems are promising: the artificial monolayer materials, like Silicene, Germanene, etc. [3, 4, 5, 6] and bilayer [7] (and in general multilayer) graphene structures. The principal distinction of the first group (we consider Silicene for definitiveness) is their buckled structure that separates A and B atoms of the honeycomb lattice in the transversal direction (Fig. 1a) and provides the required gradient of potential. As a result, the band structure can be controlled by electric field that tunes the gap and induces transition from a topological insulator to a band insulator [8, 9, 10, 11]. The field-provided inter-layer potential difference in bilayer graphene (Fig. 1b) also opens a gap between the conduction and the valence bands [7, 12], controllable by transistor gate.

Reduction of the lateral dimension of the discussed systems to the size of nanoscale quantum dot (QD) changes however their electronic properties leading to breakdown of the band structure and to enhancement of the role of the edge electronic states [13, 14, 15, 16, 17, 18, 19, 20, 21].

---

\*corresponding author

Email address: hazem.abdelsalam@etud.u-picardie.fr (Hazem Abdelsalam)

Preprint submitted to Superlattices and Microstructures

June 19, 2015

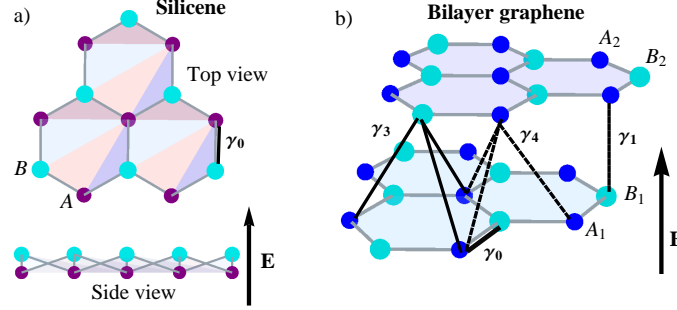


Figure 1: Structure and coupling parameters for Silicene QD (a) and for graphene bilayer QD (b).

Recent studies demonstrated that the electronic properties of QDs in graphene-type materials [22, 23] are provided by distribution of the localized edge states in the low-energy spectral region. Depending on the geometrical parameters such as size, shape, edge termination and number of layers the situation can be drastically changed from the uniformly-distributed edge-localized states to the low-energy size-quantized gap with central highly-degenerate peak of zero energy states (ZES) in the middle [23].

In this letter we investigate how the electronic states in Silicene and bilayer graphene QDs can be tuned by the transversal electric field and what impact on the future nanoscale field-effect device engineering can be expected. For calculations we use the standard tight-binding model for clusters with about 450 atoms per layer. We select the most indicative geometries of triangular and hexagonal QDs with zigzag edge termination.

## 2. Model and Density of States

The electronic properties of graphene-type materials in transversal electric field can be calculated using the tight-binding Hamiltonian [7, 5],

$$H = \sum_{\langle ij \rangle} t_{ij} c_i^\dagger c_j + \sum_i V_i(E) c_i^\dagger c_i \quad (1)$$

where  $c_i^\dagger$  and  $c_i$  are the electron creation and annihilation operators,  $t_{ij}$  are the inter-site hopping parameters and  $V_i$  is the on-site electron potential that depends both on the local atomic environment and on the applied electric field. In cases of Silicene and bilayer graphene the parameters  $t_{ij}$  can be written via the nearest neighbor (NN) coupling constants  $\gamma_i$ , as shown in Fig. 1.

Specifying Hamiltonian (1) for the case of Silicene we use the simplified version, appropriate for the low-energy states [10, 5]. In this approximation there is only one *in-plane* coupling parameter between sites A and B,  $\gamma_0 \simeq 1.6$  eV, whereas the on-site potential,  $V_i(E)$  is different for A and B sites and can be presented as  $V_i = \xi_i \Delta - \xi_i l E$  where  $\xi_i = \pm 1$  for the B and A type of atoms,  $\Delta \simeq 3.9$  meV is the effective buckling-gap parameter and  $lE$  is the field-provided electrostatic interaction, related to the up/down shift of B and A atoms on  $l \simeq 0.23$  Å with respect to the average plane.

For graphene bilayer structure, besides the *in-plane* coupling  $\gamma_0 \simeq 3.16$  eV the *interlayer* parameters  $\gamma_1 \simeq 0.38$  eV,  $\gamma_3 \simeq 0.38$  eV and  $\gamma_4 \simeq 0.14$  eV (Fig. 1b) should be also taken into

account. The field-dependent on-site potential can be written as  $V_i = \eta_i \Delta - \varsigma_i l E$  [7] where  $\eta_i = 0$  for A1 and B2 atoms,  $\eta_i = 1$  for A2 and B1 atoms and  $\varsigma_i = \pm 1$  for atoms, located in the upper (A2, B2) and lower (A1, B1) layers correspondingly (See Fig. 1). The site-environment gap parameter is taken as  $\Delta \simeq 22$  meV and the interlayer distance as  $2l \simeq 3.5$  Å.

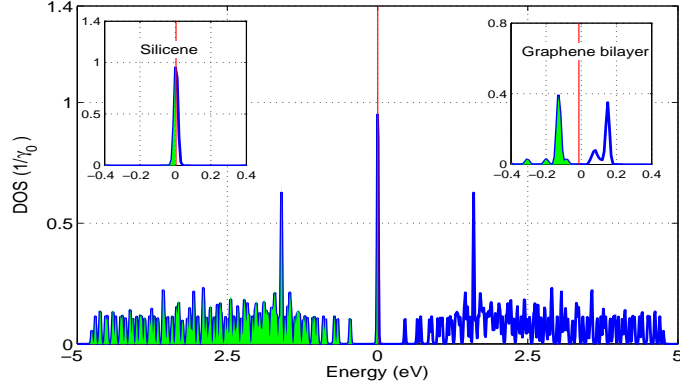


Figure 2: DOS for triangular QDs for graphene-like materials at zero field. Insets show the low-energy zoom of ZES central peaks for Silicene (left) and for Graphene bilayer (right). Here and further the vertical red line demarcates the Fermi level. The filled electronic states are shaded by green color.

The density of states (DOS) for triangular clusters of Silicene and bilayer graphene obtained at  $E = 0$  by numerical diagonalization of Hamiltonian (1) is shown in Fig. 2 where the discrete electronic levels were convoluted with Gaussian  $e^{-\epsilon^2/\delta^2}$  (with  $\delta \simeq 14$  meV  $\simeq 160$  K) that models the temperature and inhomogeneity-provided smearing. On large energy scale, the obtained DOS is similar to that for the graphene clusters [20]. The two-peak band envelope of infinite-graphene DOS is spotted by the finite-quantization cusps that vanishes with increasing of the cluster size. Most importantly, the gap in electronic states is observed at near-zero energies with sharp, almost degenerate central peak, located inside the gap. This feature is provided by the edge-localized zero energy states (ZES), that are bunched in the middle of the gap. The number of ZES,  $\eta_0$  is as large as disbalance between A and B. It reaches the maximum in case of triangular QD, for which the A-B disbalance exactly corresponds to the number of ZES and is related to the total number of atoms in QD  $N$  as  $\eta_0^\Delta = \sqrt{N+3} - 3$  [15, 17, 21]. Then, the gap is inversely proportional to  $\eta_0^\Delta$  and can be expressed via the in-plane coupling constant  $\gamma_0$  as  $2\Delta \simeq 11.12\gamma_0/\eta_0^\Delta$  [21].

The fine structures of DOS for ZES in triangular QDs of Silicene and bilayer graphene are shown on insets to Fig. 2. In Silicene, like in single-layer graphene, all ZES are concentrated exactly at zero energy, being accumulated into the highly degenerate state with degeneracy factor  $\eta_0^\Delta$ . In contrast, the central peak of ZES in bilayer graphene is smeared by the NN interlayer coupling parameter  $\gamma_4$  with formation of the finite-width double-peak structure. It is worth to note that oftenly only the non-smearing coupling  $\gamma_1$  is taken into account and constrain  $\gamma_{3,4} = 0$  is assumed. Then the splitting due to  $\gamma_4$  is overlooked and ZES is still considered to be highly degenerated.

For another QD geometries the A-B disbalance vanishes. Thus, the number of A and B atoms in hexagonal QD is equal,  $\eta_0^{hex} = 0$  and the edge-localized states are uniformly dispersed within

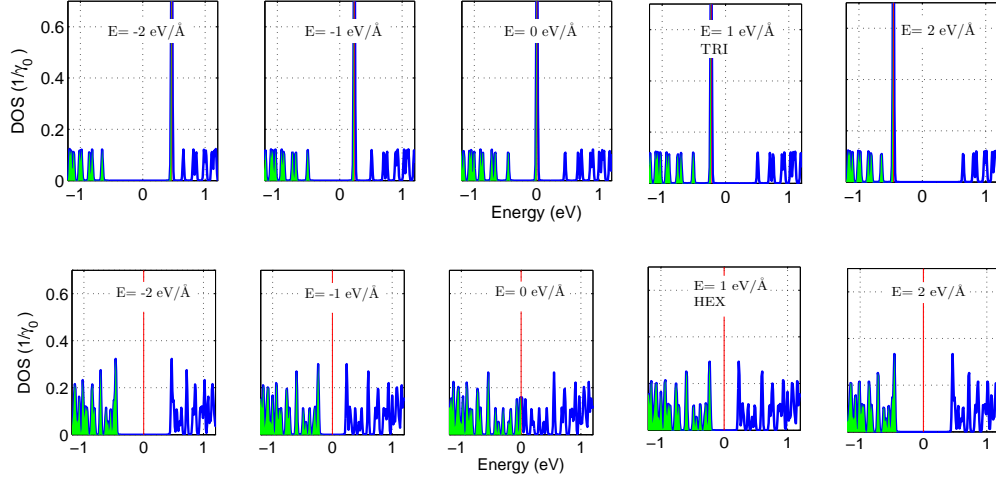


Figure 3: Evolution of ZES for triangular (upper panel) and for hexagonal (low panel) Silicene QDs as function of the applied electric field.

the size-quantized gap.

In next Chapter we shall study how these prominent features evolve with application of the electric field.

### 3. Field Tuning of Zero Energy States

#### 3.1. Silicene

Different number of up-shifted A atoms and down-shifted B atoms in triangular Silicene QD breaks the mirror cluster symmetry and results in the different reaction of QD on the up- and down-oriented electric field. The corresponding evolution of ZES under the field application (Fig. 3, upper panel) demonstrates that electric field uniformly displaces the degenerate ZES level through the gap from conducting to valence band by crossing zero energy level at  $E = 0$ . Having the Fermi level pinned by ZES peak this gives the excellent possibility to manipulate the electron interband hopping by electric field.

In contrast, the number of A and B atoms in hexagonal QD is equal and initially the size-quantized gap spectrum range is filled by dispersed ZES. Application of electric field opens the gap and symmetrically extends it to valence and conducting bands (Fig. 3, lower panel) enabling again the efficient tuning of the electronic and optical properties of the system.

#### 3.2. Bilayer graphene

Evolution of ZES in triangular QD of bilayer graphene under the action of electric field was considered in [22] where the splitting of the highly degenerate central peak on two gap-separated peaks was predicted. However, due to used in [22] approximation  $\gamma_1 \neq 0$ ,  $\gamma_{3,4} = 0$ , several relevant features were not observed. In more realistic full- $\gamma$  model, ZES are split by parameter  $\gamma_4$  already at  $E = 0$  (Fig. 2, right inset) [23] and, as demonstrated by Fig. 4, the two-smeared-peak pattern of DOS just evolves with further extension of the peak-to-peak separation (Fig. 5).

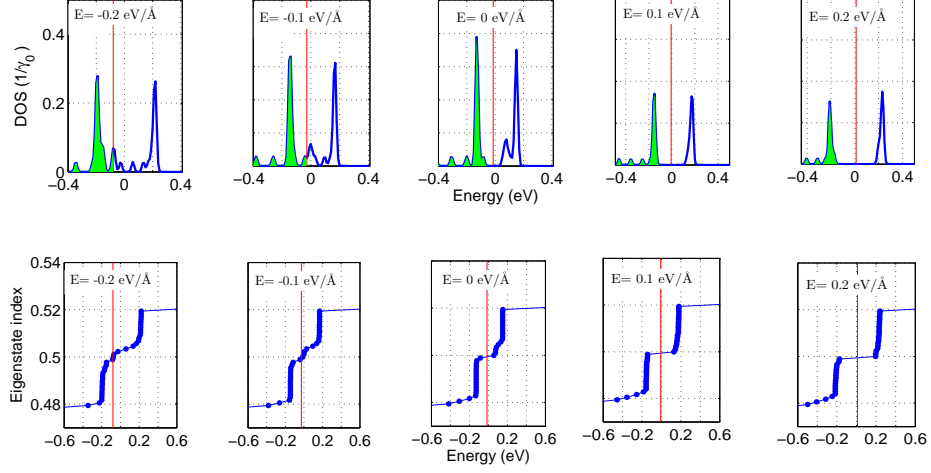


Figure 4: Evolution of DOS (upper panel) and of energy levels spectrum (lower panel) for triangular QDs of bilayer graphene as function of applied electric field in the near-zero energy region.

This peak-to-peak gap should be distinguished from the gap between the highest unoccupied electronic level (HUEL) and the lowest occupied electronic level (LOEL). The field evolution of the latter (Fig. 5) is not symmetric with respect to the field direction since not all the edge atoms in the upper plane have their  $\gamma_4$ -partners in the lower plane and the system is not perfectly symmetrical with respect to the mirror reflection.

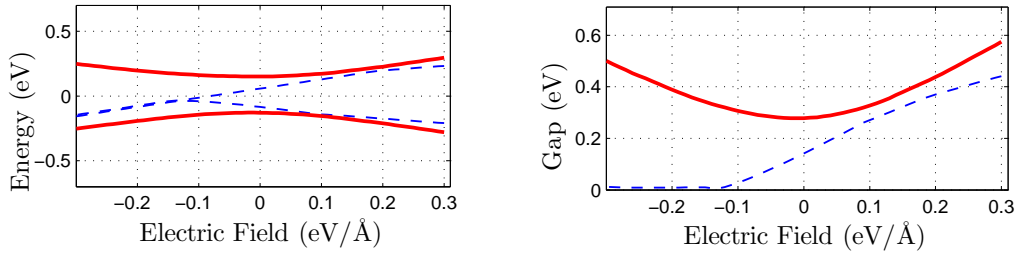


Figure 5: (left) Field dependence of peaks of splitted ZES in bilayer graphene (red solid line) and of LOEL and HUEL energies (dashed blue lines). (right) Corresponding field dependence of peak-to-peak and LOEL-HUEL gaps.

#### 4. Discussion

Described above possibility of field-manipulation by electronic properties of Silicene and bilayer graphene QDs is provided by the field-dependent distribution of the edge-localized ZES

inside the size-quantized gap and therefore is quite different from the suggested previously mechanism of the band-gap tuning in the bulk state [3, 7, 12, 8]. Moreover, as can be seen from the previous section, the evolution of ZES is very sensitive to sample geometry. This certainly creates the wealth of possibilities for design of QDs with required tunable electronic parameters but poses the query concerning their stability with respect to the cluster shape change. The fortunate answer is coming from analysis of the factors affecting ZES behavior. Whereas the value size-quantized gap with ZES in the middle depends on QD dimensions, the HUEL-LOEL separation, provided by sporadic distribution of individual levels, is just the function of structure of the edge termination. More importantly however that such remarkable effects as (i) field-provided displacement of central peak in triangular Silicene QD, (ii) field-induced gap in quasi-continuum edge-localized-states spectrum in hexagonal Silicene QD and (iii) field evolution of peak-to-peak gap splitting of ZES in bilayer graphene QD are caused by the inter-plane coupling parameters  $\gamma_i$  and therefore are less sensitive to the geometry variation. Our numerical calculations indeed demonstrate the perfect scalability of these properties, making them a universal feature valid even for ensemble of similar-shape clusters.

Tight-binding calculations presented here do not take into account the cooperative Coulomb electron correlations [22] and another gap-generating effects, like e.g. doping [24], vacuum fluctuations [25] etc. Full account of these effects under the action of tuning field is the challenging problem. Another interesting problem is the evolution of the energy spectrum under the influence of both electric and magnetic field, especially if the last one exceeds the quantum limit. Generalization of obtaining results for the multilayer carbon clusters can possibly be useful to explain the unconventional tiny magnetic properties of graphite in the ultra-quantum regime [26].

This work was supported by the Egyptian mission sector and by the European mobility FP7 Marie Curie program ITN-NOTEDDEV.

## References

- [1] Z. Ni, H. Zhong, X. Jiang, R. Quhe, G. Luo, Y. Wang, M. Ye, J. Yang, J. Shi, and J. Lu, *Nanoscale* **6** (2014) 7609.
- [2] L. Tao, E. Cinquanta, D. Chiappe, C. Grazianetti, M. Fanciulli, M. Dubey, A. Molle, and D. Akinwande *Nature Tech.* **96** (2015) 227.
- [3] W. -F. Tsai, C. -Y. Huang, T. -R. Chang, H. Lin, H. -T. Jeng, and A. Bansil, *Nature Commun.* **4** (2013) 1500.
- [4] E. Bianco, S. Butler, S. Jiang, O. D. Restrepo, W. Windl and J. E. Goldberger, *ACS Nano.* **7** (2013) 4414.
- [5] C. -C Liu, H. Jiang and Y. Yao, *Phys. Rev. B* **84** (2011) 195430.
- [6] F. Bechstedt, L. Matthes, P. Gori, O. Pulci, *Appl. Phys. Lett.* **100** (2012) 261906.
- [7] E. McCann and M. Koshino, *Rep. Prog. Phys.* **76** (2013) 056503.
- [8] C. -C Liu, W. Feng and Y. Yao, *Phys. Rev. Lett.* **107** (2011) 076802.
- [9] N. D. Drummond, V. Zolyomi, and V. I. Falko, *Phys. Rev. B* **85** (2012) 075423.
- [10] M. Ezawa, *New J. Phys.* **14** (2012) 033003.
- [11] V. Yu. Tsaran and S. G. Sharapov, *Phys. Rev. B* **90** (2014) 205417.
- [12] E. V. Castro, K. S. Novoselov, S. V. Morozov, N. M. R. Peres, J. M. B. Lopes dos Santos, J. Nilsson, F. Guinea, A. K. Geim, and A. H. Castro Neto, *Phys. Rev. Lett.* **99** (2007) 216802.
- [13] M. Ezawa, *Phys. Rev. B* **76** (2007) 245415.
- [14] Z. Z. Zhang, K. Chang, and F. M. Peeters, *Phys. Rev. B* **77** (2008) 235411.
- [15] J. Fernandez-Rossier and J. J. Palacios, *Phys. Rev. Lett.* **99** (2007) 177204.
- [16] W. L. Wang, O. V. Yazyev, S. Meng, and E. Kaxiras, *Phys. Rev. Lett.* **102** (2009) 157201.
- [17] P. Potasz, A. D. Guclu, and P. Hawrylak, *Phys. Rev. B* **81** (2010) 033403.
- [18] C. A. Downing, D. A. Stone, and M. E. Portnoi, *Phys. Rev. B* **84** (2011) 155437.
- [19] M. Zarenia, A. Chaves, G. A. Farias, and F. M. Peeters, *Phys. Rev. B* **84** (2011) 245403.
- [20] T. Espinosa-Ortega, I. A. Luk'yanchuk, and Y. G. Rubo, *Superlattices Microstruct.* **49** (2011) 283.
- [21] T. Espinosa-Ortega, I. A. Luk'yanchuk, and Y. G. Rubo, *Phys. Rev. B* **87** (2013) 205434.
- [22] A. D. Guclu, P. Potasz, and P. Hawrylak, *Phys. Rev. B* **84** (2011) 035425.
- [23] H. Abdelsalam, T. Espinosa-Ortega, I. Lukyanchuk, *Low Temp. Phys. in Print* (2015); (arXiv:1412.8351).

- [24] J. E. Barrios-Vargas, G. G. Naumis, Solid State Communications, **162** (2013) 23.
- [25] O. V. Kibis, O. Kyriienko, I. A. Shelykh, Phys. Rev. B **84** (2011) 195413.
- [26] Y. Kopelevich, B. Raquet, M. Goiran, W. Escoffier, R. R. da Silva, J. C. Medina Pantoja, I. A. Lukyanchuk, A. Sinchenko, and P. Monceau, Phys. Rev. Lett. **103** (2009) 116802.